EOS7, An Equation-of-State Module for the TOUGH2 Simulator for Two-Phase Flow of Saline Water and Air

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Introduction

In studies of geothermal reservoirs and nuclear waste repositories one frequently encounters flow systems with an aqueous phase of variable salinity. In addition, non-condensible gas(es) may be present or may be generated, which are soluble in the aqueous phase to some extent, but which will exsolve to form a free gas phase at sufficiently high concentrations. In order to model fluid and heat flow in such systems, it is necessary to provide a representation of the thermophysical properties of the fluid mixtures as a function of suitable primary thermodynamic variables. EOS7 describes the main effects of salinity, including the density and viscosity of the aqueous phase, and the dependence of gas solubility on salinity. The present version of EOS7 neglects effects of salinity on enthalpy and vapor pressure of the aqueous phase, and also neglects possible changes in capillary pressures and relative permeabilities from composition-dependent surface tension.

Scope and Methodology

An extension of the "EOS3" module of TOUGH2 for water/air mixtures, EOS7 represents the aqueous phase as a mixture of a "concentrated" (not necessarily saturated) brine and pure water. This follows similar treatments by Reeves *et al.* (1986) and Herbert *et al.* (1988). Quantitatively, the saline mixture is described as consisting of a mass fraction X_b of brine, and a mass fraction $X_w = (1 - X_b)$ of water. The brine is modeled as NaCl solution, while the non-condensible gas is air, although the treatment can be adapted, with minor modifications, to other salts and gases. The representation of the temperature and pressure dependence of thermophysical properties is somewhat more general than that of Reeves *et al.* (1986), retaining the flexibility of the TOUGH2 formulation for nonisothermal processes. However, the accuracy of our formulation for systems with a broad range of fluid temperatures, such as hydrothermal convection systems, has not yet been evaluated. Therefore, EOS7 should be used with caution when dealing

with systems that involve a large range of fluid temperatures. For systems with limited temperature variations, of order 10–30°C, the description of the temperature and pressure dependence of the aqueous phase density in EOS7 will essentially reduce to the approach of Reeves *et al.* (1986).

EOS7 can describe flow regions in single-phase liquid and two-phase conditions. A general capability for single-phase gas would require the description of salt precipitation from vaporizing brines, with associated porosity and permeability effects, which is outside the scope of the water-brine mixing model adopted in EOS7. We have provided a "rudimentary" description of single-phase gas conditions, that does not allow for any solid phase to form. Properly speaking, brine concentration in the gas phase should vanish. However, in a phase transition from two-phase conditions with brine present in the liquid phase to single-phase gas conditions, it would be impossible to satisfy the brine mass balance if gas phase brine mass fraction were held to zero. (Drying up of two-phase conditions would of course result in the salt being deposited as a solid phase.) In making a transition from two-phase to single-phase gas conditions, we therefore initialize $X_b = 0$ in the gas phase, but permit X_b to vary freely until convergence of all mass and heat balance equations is attained. Thus, non-zero values for brine mass fraction may arise in the gas phase. However, for physically meaningful solutions, X_b should always remain "very small" in single-phase gas conditions, and computed results should be closely monitored to make sure that this is the case.

Another limitation is that TOUGH2, Version 1.0, does not include a description of dispersion or diffusion in the liquid phase. Thus, relative movement of brine and water occurs only through advection and through numerical dispersion, which is an artefact of space and time discretization.

We shall now summarize the treatment adopted for the different thermophysical properties.

Liquid Density

According to data presented by Herbert *et al.* (1988), the mixing of water with a (concentrated or dilute) salt solution results in a total fluid volume that is very close to the sum of water and salt solution volumes (data for NaCl solutions at T = 20°C, P = 1 atm). Denoting water and brine volumes by V_w and V_b, respectively, the mixture volume is given, to a very good approximation, by

$$V_m = V_w + V_b \tag{1}$$

The mass of the mixture is

$$M_m = M_w + M_b \tag{2}$$

and mass fractions of brine and water are given by

$$X_b = \frac{M_b}{M_m} \tag{3a}$$

$$X_w = 1 - X_b \tag{3b}$$

Dividing Eq. (1) by (2) and inserting from (3) we have for the mixture density

$$\frac{1}{\rho_m} = \frac{V_m}{M_m} = \frac{1 - X_b}{\rho_w} + \frac{X_b}{\rho_b} \tag{4}$$

where $\rho_w = M_w/V_w$ and $\rho_b = M_b/V_b$. The mixing rule Eq. (4) applies to the concentration dependence of mixture density at conditions of constant temperature and pressure. In order to achieve a simple approximate representation of mixture density for variable temperature and pressure, we make the assumption that the expansivity and compressibility of brine is independent of salinity and equal to the values for pure water at all temperatures and pressures. This approximation will provide reasonable values for brine density at least over a limited range of temperatures and pressures around reference conditions (P_0, T_0). Thus the relative change of density as function of temperature and pressure for brine is the same as for pure water:

$$\frac{\rho_b(P,T)}{\rho_b(P_0,T_0)} = \frac{\rho_w(P,T)}{\rho_w(P_0,T_0)} \tag{5}$$

To calculate mixture density at arbitrary temperature, pressure, and concentration we use Eq. (5) for brine density in Eq. (4). The default reference brine has a density of 1185.1 kg/m^3 at reference conditions of $P_0 = 1$ bar, $T_0 = 25°C$, corresponding to an NaCl solution of 24.98 wt-% or 5.06 molar (Potter et al., 1977, cited after Finley and Reeves, 1982). Different reference conditions and brine densities may be specified by the user so that, for limited variations of pressure and temperature, our approach becomes similar to the first-order expansion in pressure and temperature used by Reeves et al. (1986). The representation of salinity dependence in Eq. (4) follows the more general formulation of Herbert et al. (1988), which is expected to retain excellent accuracy even for very large salinity variations.

Liquid Viscosity

Following Herbert et al. (1988), salinity effects on aqueous phase viscosity are modeled with a polynomial correction to the viscosity of pure water. Mixture viscosity is represented as follows.

$$\mu_m(P, T, X_b) = \mu_w(P, T) \cdot f(X_b) \tag{6}$$

where

$$f(X_b) = 1 + v(1) \cdot X_b + v(2) \cdot X_b^2 + v(3) \cdot X_b^3 \tag{7}$$

with default values of $v(1) = 0.4819$, $v(2) = -0.2774$ and $v(3) = 0.7814$. Different values for the coefficients may be specified by the user.

Gas Solubility

According to Henry's law, the mole fraction x_a of air dissolved in liquid water is proportional to the partial pressure P_a of air.

$$x_a = (1/K_h) \cdot P_a \tag{8}$$

K_h is Henry's constant, which is a slowly varying function of temperature, varying from 6.7×10^9 Pa at 20°C to 1.0×10^{10} Pa at 60°C and 1.1×10^{10} Pa at 100°C (Loomis, 1928). Because air solubility is small, such a moderate variation was not expected to cause significant effects, and a constant value of $K_h = 1.0 \times 10^{10}$ Pa was adopted in EOS3 of TOUGH2.

In saline solutions most gases are less soluble than in pure water (''salting out'' effect). For a 5N NaCl solution, nitrogen solubility is virtually independent of temperature in the range 0°C < T < 100°C, and corresponds to a Henry's constant of 4.0×10^{10} Pa (Cygan, 1991). We retain the value of $K_h = 1.0 \times 10^{10}$ for pure water, and represent air solubility (inverse of Henry's constant) as a linear function of mixture molarity, as follows.

$$\left[\frac{1}{K_h} \right]_m = 1.0 \times 10^{-10} + \left[\frac{N_m}{5} \right] \left[\frac{1}{4.0 \times 10^{10}} - 10^{-10} \right] \tag{9}$$

Mixture molarity is calculated from the density ρ_b and molarity N_b of the reference brine.

$$N_m = X_b N_b \frac{\rho_m}{\rho_b} \tag{10}$$

Application of EOS7

EOS7 is compatible with TOUGH2, Version 1.0, and can be used in completely analogous fashion to the EOS modules EOS1 through EOS5 described in the TOUGH2 report (Pruess, 1991). A summary of EOS7 specifications and options is printed upon program execution, and is here reproduced in Figure 1. A number of options is available to increase calculational efficiency for certain types of flow problems. By means of appropriate specifications in the ''MULTI'' data block of TOUGH2, it is possible to run EOS7 in two-component mode (NK=2), which represents only water-brine mixtures without air. Both two- and three-component options can be run in

isothermal mode; the energy equation can be disregarded by simply specifying NEQ = NK (= 2 or 3), instead of the fully nonisothermal mode NEQ = NK+1. Computational work is typically proportional to the square of the number of equations solved per grid block, so that these options, where applicable, can result in substantial savings in computer time. Even when no energy equation is solved, temperature must still be specified and can in fact be variable throughout the grid system; however, initial temperatures will remain unchanged during a simulation run when the NEQ=NK option is chosen.

Injection of different fluid components can be specified by setting character variable TYPE in block GENER equal to 'COM1', 'COM2' or 'COM3', respectively, for water, brine or air.

A separate data block with keyword "SELEC" is used for optional specification of reference brine data by the user. This block can appear anywhere (between data blocks) in the TOUGH2 input file and consists of the following records (see Figure 2).

SELEC   keyword to introduce a data block with optional reference brine data

SELEC.1 Format(I5)

         IE(1)

         IE(1)   set equal to 2, to read two additional data records (in future versions of EOS7, more additional data records may be read, e.g., to provide tabular input for thermophysical properties; larger values of IE(1) would then be used)

SELEC.2   Format(3E10.4)

         P_0, T_0, ρ_b

         P_0 reference pressure, in Pa

         T_0 reference temperature, in °C

         ρ_b brine density at (P_0,T_0), in kg/m^3

         For P_0, T_0 and ρ_b equal to zero or blank, default values of $P_0 = 1 \times 10^5$ Pa, $T_0 = 25$°C, $\rho_b = 1185.1$ kg/m^3 will be used. For $P_0 < 0$, brine will be assumed to be pure water. This allows modeling of flow with two waters that differ only in trace constituents, but have identical thermophysical properties.

SELEC.3   Format(3E10.4)

         v(i),i=1,3

v(i)   coefficients for salinity correction in aqueous phase viscosity (see Eq. 7). If v(i) = 0 for i = 1, 2, 3, default values will be used: v(1) = 0.4819, v(2) = − 0.2774, v(3) = 0.7814. Specification of brine as pure water in record SELEC.2 will override viscosity specifications, and will always result in viscosity of pure water being used.

Sample Problem

Figures 3 through 7 show specifications and some results for a simulation problem that involves nonisothermal flow of variably saline brine and air. The problem was not designed with a single "real-life" flow problem in mind; rather, the purpose is to illustrate implementation of a variety of thermodynamic conditions and generation options, and to provide a benchmark for proper code implementation.

The input file (see Figure 3) has MESHMAKER specifications for a three-dimensional $5 \times 5 \times 2$ X-Y-Z mesh. The grid blocks are cubes of 1 m^3 volume. Figure 4 shows the mesh pattern printout generated by the TOUGH2 run. Grid block names start with "A1" in the top layer and with "A2" in the bottom layer. Data block "SELEC" chooses default parameters for the reference brine, and "MULTI" specifies that the 3-component option (water, brine, air) is to be used in nonisothermal mode (NK = 3, NEQ = 4).

Default initial conditions are (last record in data block "PARAM"): Pressure P = 10^5 Pa, brine mass fraction X_b = 0.5, air mass fraction X = 0., and temperature T = 25°C. Various different initial conditions are chosen for portions of the flow domain in block "INCON". In the top layer, the first row of grid blocks (A11 1 through A11 5) has X_b = 0., corresponding to single-phase water without salinity; the middle row (A13 1 through A13 5) has X_b = 0., X = 0.99, corresponding to single-phase gas conditions; the bottom row (A15 1 through A15 5) is initialized with X_b = 1., corresponding to pure brine. In the bottom layer, various two-phase conditions with 50% gas saturation are prescribed for grid blocks in the middle row. In A23 1 and A23 2 the aqueous phase is pure water, in A23 3 it has 50% brine mass fraction, and in A23 4 and A23 5 it is 100% brine.

Generation options include a "well" on deliverability in the upper left corner of the grid (block A11 1), brine injection ("COM2") in the upper right corner (block A11 5), water injection ("COM1") in the lower right corner (block A25 5), heat generation in the center block of the lower layer (A23 3), and air injection ("COM3") in the lower left corner (block A25 1). Brine enthalpy is 10^6 J/kg, corresponding to a temperature of approximately 233°C, while enthalpy of injected water, 3×10^5 J/kg, corresponds to a temperature of approximately 72°C. Air is injected at lower rate (10^{-4} kg/s) and enthalpy (2×10^5 J/kg). Air specific heat at constant pressure is

approximately 1010 J/kg°C (Vargaftik, 1975), so that this enthalpy corresponds to a temperature of approximately 198°C.

Figure 5 gives a portion of the printout from the TOUGH2 run after the first "infinitesimal" time step of 10^{-9} seconds. This small initial time step was chosen deliberately to obtain convergence at unaltered initial conditions. The printout was edited, keeping only seven grid blocks to show data for each of the seven different initial conditions specified. The iteration sequence for time step #2 with $\Delta t = 2$ seconds and a portion of the printout after two time steps are shown in Figure 6. The strong suction pressures in the single-phase gas blocks have drawn enough aqueous phase to effect a transition to two-phase conditions there (blocks A13 1 through A13 5). The liquid inflow results in a pressure increase which is very small due to the very large compressibility of gas (approximately $1/P = 10^{-5}$ Pa^{-1}), while pressure drop in the blocks initially in single-phase liquid conditions is large due to the small compressibility of liquid water (of order 10^{-10} Pa^{-1}). Gas phase, mostly air with a small fraction of water vapor, flows from the blocks that were initially in single-phase gas or two-phase conditions into the neighboring single-phase liquid blocks, causing phase transitions to two-phase conditions there. The air injection block A25 1 remains in single-phase liquid conditions, because the amount of air injected in 2 seconds is below the solubility limit at prevailing pressures. Note that brine mass fraction in A13 1 is smaller than in A13 5, reflecting different aqueous phase compositions in the neighboring blocks that provide the liquid inflows.

With automatic time step control, total desired simulation time of 86,400 seconds (1 day) is reached after 52 time steps. Results are shown in Figure 7. Most of the flow system, except for the vicinity of the block receiving water injection, is now in two-phase conditions. Air is the dominant gas phase component in the cooler regions, while vapor dominates in the hotter regions. Aqueous phase compositions vary over a broad range. X_b exceeds 1 in a few grid blocks, representing a salinity in excess of the reference brine. This effect is due to partial vaporization, which increases the salinity of the residual aqueous phase. Fluid production rate from A11 1 exceeds rate of mass injection, reflecting additional fluid expulsion from rising temperatures. Only approximately 0.1 wt-% of production occurs as gas phase.

The volume and mass balances (Figure 7) indicate that gas phase volume has decreased in the course of the simulation, while mass present in the gas phase has increased by more than a factor 3, reflecting the considerable overall pressurization of the flow system.

On a Cray X-MP computer, the simulation required a CPU time of 56.3 seconds.

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Figure Captions

Figure 1.   Summary of EOS7 specifications and options.

Figure 2.   Input formats for data block "SELEC".

Figure 3.   TOUGH2 input file for EOS7 test problem.

Figure 4.   TOUGH2 printout of mesh pattern for sample problem.

Figure 5.   Some output data after first time step.

Figure 6.   Iteration sequence and portion of output after time step 2.

Figure 7.   TOUGH2 output after 1 day of simulation time.

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*********************************************************************************************************************
*                        EOS7: EQUATION OF STATE FOR MIXTURES OF WATER/BRINE/AIR                                    *
*********************************************************************************************************************


    OPTIONS SELECTED ARE: (NK,NEQ,NPH,NB) = (3,4,2, 6)

                        NK  = 3   - NUMBER OF FLUID COMPONENTS
                        NEQ = 4   - NUMBER OF EQUATIONS PER GRID BLOCK
                        NPH = 2   - NUMBER OF PHASES THAT CAN BE PRESENT
                        NB  = 6   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN COMPONENT MASS FRACTIONS)


    AVAILABLE OPTIONS ARE: (NK,NEQ,NPH,NB) = (3,3,2,6) - WATER, BRINE, AIR; ISOTHERMAL (DEFAULT); VARIABLES (P, XB, X OR S+10, T)
                                             (3,4,2,6) - WATER, BRINE, AIR; NON-ISOTHERMAL;        VARIABLES (P, XB, X OR S+10, T)
                                             (2,2,2,6) - WATER, BRINE, NO AIR; ISOTHERMAL;         VARIABLES (P, XB, T)
                                             (2,3,2,6) - WATER, BRINE, NO AIR; NON-ISOTHERMAL;     VARIABLES (P, XB, T)

    THE NK = 2 ("NO AIR") OPTIONS MAY ONLY BE USED FOR PROBLEMS WITH SINGLE-PHASE LIQUID CONDITIONS THROUGHOUT


*********************************************************************************************************************

THE PRIMARY VARIABLES ARE
 P - PRESSURE          T - TEMPERATURE        X - AIR MASS FRACTION        S+10. - (GAS PHASE SATURATION + 10.)
XB - BRINE MASS FRACTION IN LIQUID (EXCEPT FOR SINGLE-PHASE GAS, WHERE XB IS BRINE MASS FRACTION IN GAS)

*********************************                      ********************************************************
*        COMPONENTS          *                        *   FLUID PHASE CONDITION       PRIMARY VARIABLES      *
*********************************                      ********************************************************
*                            *                        *                                                     *
*     # 1  -  WATER          *                        *   SINGLE-PHASE GAS (#)       P,    XB,      X,    T  *
*                            *                        *                                                     *
*     # 2  -  BRINE          *                        *   SINGLE-PHASE LIQUID        P,    XB,      X,    T  *
*                            *                        *                                                     *
*     # 3  -  AIR            *                        *   TWO-PHASE                  P,    XB,   S+10.,   T  *
*                            *                        *                                                     *
*     # 4  -  HEAT           *                        ********************************************************
*                            *                              (#) SINGLE-PHASE GAS NOT FULLY IMPLEMENTED
*********************************************************************************************************************

BRINE PROPERTIES
            DENSITY = 0.118510E+04 KG/M**3 AT REFERENCE CONDITIONS OF (P,T) = (0.100000E+06 PA,0.250000E+02 DEG-C)
            COEFFICIENTS FOR BRINE VISCOSITY ARE: VCO(I) = 0.481900E+00 -.277400E+00 0.781400E+00


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Figure 1.   Summary of EOS7 specifications and options.

Figure 2.   Input formats for data block "SELEC".

```
*RF1*  ... EOS7-TEST: INJECT AIR, HEAT, BRINE AND FRESH WATER
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ

NX        5        1.
NY        5        1.
NZ        2        1.


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
POMED     2650.            .25  200.E-15  200.E-15  200.E-15        2.2      1000.

.....USE DEFAULT PARAMETERS FOR REFERENCE BRINE
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     2


.....SPECIFY THREE COMPONENTS (WATER, BRINE, AIR); SOLVE ENERGY EQUATION
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     3    4    2    6
START
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  99    9910000000000002 47
0.          8.64E4        -1.                              9.81
     1.E-9        2.
     1.E-5        1.
                 1.E5                  0.5                 0.0                 25.
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     1          .30      .05      1.        1.
     1          5.E5     .20      1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
     3    3
     1.E-9        2.   8.64E4
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1PRO 1                      DELV     2.E-13    1.E5
A11 5BRI 1                      COM2     5.E-2     1.E6
A25 5WTR 1                      COM1     5.E-2     3.E5
A23 3HOT 1                      HEAT     1.E5
A25 1AIR 1                      COM3     1.E-4     2.E5

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1    4    1
                 1.E5            0.00                 0.0                 25.
A13 1    4    1
                 1.E5            0.00                 0.99                25.
A15 1    4    1
                 1.E5            1.0                  0.0                 25.
A23 1    1    1
                 1.E5            0.00                 10.50               25.
A23 3
                 1.E5            0.50                 10.50               25.
A23 4    1    1
                 1.E5            1.0                  10.50               25.

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 3.   TOUGH2 input file for EOS7 test problem.

```
!*******************************************************************************************************************
*                    CARTESIAN MESH WITH NX*NY*NZ =    5 *   5 *   2 GRID BLOCKS                                   *
*******************************************************************************************************************
*                                                                                                                 *
*                    THE MESH WILL BE PRINTED AS SLICES FOR K = 1 TO K = NZ =   2                                  *
*                                                                                                                 *
*                    IN EACH MESH SLICE, ROWS WILL GO FROM  J = 1 TO J = NY =   5                                  *
*                                                                                                                 *
*                    IN EACH ROW, COLUMNS WILL GO FROM      I = 1 TO I = NX =   5                                  *
*                                                                                                                 *
*******************************************************************************************************************

SLICE WITH K =   1

  COLUMN I = 1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16   17   18   19   20
ROWS
 J =   1    A11 1 A11 2 A11 3 A11 4 A11 5
 J =   2    A12 1 A12 2 A12 3 A12 4 A12 5
 J =   3    A13 1 A13 2 A13 3 A13 4 A13 5
 J =   4    A14 1 A14 2 A14 3 A14 4 A14 5
 J =   5    A15 1 A15 2 A15 3 A15 4 A15 5
*******************************************************************************************************************

SLICE WITH K =   2

  COLUMN I = 1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16   17   18   19   20
ROWS
 J =   1    A21 1 A21 2 A21 3 A21 4 A21 5
 J =   2    A22 1 A22 2 A22 3 A22 4 A22 5
 J =   3    A23 1 A23 2 A23 3 A23 4 A23 5
 J =   4    A24 1 A24 2 A24 3 A24 4 A24 5
 J =   5    A25 1 A25 2 A25 3 A25 4 A25 5

*******************************************************************************************************************

MESH GENERATION COMPLETE --- EXIT FROM MODULE *MESHMAKER*
```

Figure 4.   TOUGH2 printout of mesh pattern for sample problem.

RF1 ... EOS7-TEST: INJECT AIR, HEAT, BRINE AND FRESH WATER

OUTPUT DATA AFTER (1, 1)-2-TIME STEPS   THE TIME IS 0.115741E-13 DAYS

0@@

TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
0.100000E-08	1	1	1	2	0.	0.	0.	0.10720E-09	5	1	0.10000E-08

0@@

OELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XBRINE(LIQ)	XAIRG	XAIRL	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
A11 1	1	0.10000E+06	0.25000E+02	0.	0.10000E+01	0.	0.	0.	0.	0.	0.99716E+03
A21 1	2	0.10000E+06	0.25000E+02	0.	0.10000E+01	0.50000E+00	0.	0.	0.	0.	0.10830E+04
.....											
.....											
A13 1	5	0.10000E+06	0.25000E+02	0.10000E+01	0.	0.	0.99000E+00	0.	-.50000E+06	0.11612E+01	0.
A23 1	6	0.10000E+06	0.25000E+02	0.50000E+00	0.50000E+00	0.	0.98004E+00	0.15566E-04	-.31250E+06	0.11543E+01	0.99716E+03
.....											
.....											
A15 1	9	0.10000E+06	0.25000E+02	0.	0.10000E+01	0.10000E+01	0.	0.	0.	0.	0.11851E+04
.....											
.....											
A23 3	26	0.10000E+06	0.25000E+02	0.50000E+00	0.50000E+00	0.50000E+00	0.98004E+00	0.10167E-04	-.31250E+06	0.11543E+01	0.10830E+04
.....											
.....											
A23 4	36	0.10000E+06	0.25000E+02	0.50000E+00	0.50000E+00	0.10000E+01	0.98004E+00	0.37513E-05	-.31250E+06	0.11543E+01	0.11851E+04
.....											
.....											

********* VOLUME- AND MASS-BALANCES ***

********* [KCYC,ITER] = [1, 1] *****   THE TIME IS 0.100000E-08 SECONDS, OR 0.115741E-13 DAYS

PHASE VOLUMES IN PLACE
GAS 0.187500E+01 M**3;   LIQUID 0.106250E+02 M**3

MASS IN PLACE
GAS 0.217290E+01 KG;   LIQUID 0.115315E+05 KG;   BRINE 0.590673E+04 KG;   VAPOR 0.289151E-01 KG;   TOTAL WATER 0.562484E+04 KG
AIR 0.215035E+01 KG

TOTAL BRINE MASS IN SINGLE-PHASE GAS REGIONS IS 0.   KG

****

Figure 5.   Some output data after first time step.

```
...ITERATING... AT [  2,  1] --- DELTEX = 0.200000E+01   MAX. RES. = 0.214398E+00  AT ELEMENT A13 1  EQUATION   1
...ITERATING... AT [  2,  2] --- DELTEX = 0.200000E+01   MAX. RES. = 0.237418E+01  AT ELEMENT A13 5  EQUATION   1
...ITERATING... AT [  2,  3] --- DELTEX = 0.200000E+01   MAX. RES. = 0.150830E+00  AT ELEMENT A13 4  EQUATION   2
...ITERATING... AT [  2,  4] --- DELTEX = 0.200000E+01   MAX. RES. = 0.296492E-01  AT ELEMENT A13 5  EQUATION   2
...ITERATING... AT [  2,  5] --- DELTEX = 0.200000E+01   MAX. RES. = 0.386808E-03  AT ELEMENT A13 5  EQUATION   2
A13 5(  2,  6) ST = 0.200000E+01 DT = 0.200000E+01 DX1= 0.769778E+03 DX2= 0.523168E+00 T =  24.997 P =   100770.  S = 0.998704E+00


*RF1* ... EOS7-TEST: INJECT AIR, HEAT, BRINE AND FRESH WATER

        OUTPUT DATA AFTER (  2,  6)-2-TIME STEPS                              THE TIME IS 0.231481E-04 DAYS

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  TOTAL TIME   KCYC  ITER  ITERC   KON       DX1M        DX2M        DX3M         MAX. RES.      NER    KER      DELTEX
  0.200000E+01   2    6     7      2      0.69558E+05 0.52319E+00 0.10009E+02     0.67308E-07    45     2     0.20000E+01

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@ELEM.  INDEX    P          T          SG         SL       XBRINE(LIQ) XAIRG      XAIRL      PCAP        DG         DL
                (PA)      (DEG-C)                                                           (PA)      (KG/M**3)  (KG/M**3)

 A11 1    1 0.52527E+05 0.25000E+02 0.          0.10000E+01 -.10334E-18 0.         0.         0.         0.         0.99714E+03
 A21 1    2 0.55216E+05 0.25000E+02 0.          0.10000E+01 0.49999E+00 0.         0.         0.         0.         0.10830E+04
 A12 1    3 0.47184E+05 0.25000E+02 0.63001E-03 0.99937E+00 0.49999E+00 0.95712E+00 0.46218E-05 -.39376E+03 0.53727E+00 0.10830E+04
 A22 1    4 0.30442E+05 0.25000E+02 0.23628E-03 0.99976E+00 0.50000E+00 0.93257E+00 0.28639E-05 -.14767E+03 0.34169E+00 0.10830E+04
 A13 1    5 0.10077E+06 0.24997E+02 0.99866E+00 0.13406E-02 0.47280E+00 0.98020E+00 0.10568E-04 -.50000E+06 0.11633E+01 0.10780E+04
 A23 1    6 0.99068E+05 0.25000E+02 0.49940E+00 0.50060E+00 0.74696E-03 0.97985E+00 0.15408E-04 -.31213E+06 0.11434E+01 0.99728E+03
 A14 1    7 0.47182E+05 0.25000E+02 0.63115E-03 0.99937E+00 0.50000E+00 0.95711E+00 0.46215E-05 -.39447E+03 0.53724E+00 0.10830E+04
 A24 1    8 0.30442E+05 0.25000E+02 0.23631E-03 0.99976E+00 0.50000E+00 0.93257E+00 0.28639E-05 -.14770E+03 0.34169E+00 0.10830E+04
 A15 1    9 0.56908E+05 0.25000E+02 0.          0.10000E+01 0.10000E+01 0.         0.65077E-22 0.         0.         0.11851E+04
 A25 1   10 0.55194E+05 0.25000E+02 0.          0.10000E+01 0.50001E+00 0.         0.73865E-06 0.         0.         0.10830E+04
 .....
 .....
 A11 5   41 0.12723E+06 0.25030E+02 0.          0.10000E+01 0.40098E-03 0.         0.67491E-23 0.         0.         0.99723E+03
 A21 5   42 0.85087E+05 0.25000E+02 0.          0.10000E+01 0.49996E+00 0.         0.         0.         0.         0.10830E+04
 A12 5   43 0.47490E+05 0.25000E+02 0.49800E-03 0.99950E+00 0.49993E+00 0.95740E+00 0.46542E-05 -.31125E+03 0.54084E+00 0.10830E+04
 A22 5   44 0.30524E+05 0.25000E+02 0.19398E-03 0.99981E+00 0.50000E+00 0.93276E+00 0.28725E-05 -.12124E+03 0.34264E+00 0.10830E+04
 A13 5   45 0.10077E+06 0.24997E+02 0.99870E+00 0.12963E-02 0.52317E+00 0.98020E+00 0.99732E-05 -.50000E+06 0.11633E+01 0.10874E+04
 A23 5   46 0.99071E+05 0.25000E+02 0.49936E+00 0.50064E+00 0.99937E+00 0.97985E+00 0.37241E-05 -.31210E+06 0.11434E+01 0.11850E+04
 A14 5   47 0.47276E+05 0.25000E+02 0.59084E-03 0.99941E+00 0.50002E+00 0.95720E+00 0.46312E-05 -.36928E+03 0.53834E+00 0.10830E+04
 A24 5   48 0.30742E+05 0.25000E+02 0.83035E-04 0.99992E+00 0.50000E+00 0.93325E+00 0.28954E-05 -.51897E+02 0.34519E+00 0.10830E+04
 A15 5   49 0.10152E+06 0.25000E+02 0.          0.10000E+01 0.99997E+00 0.         0.         0.         0.         0.11851E+04
 A25 5   50 0.16486E+06 0.25006E+02 0.          0.10000E+01 0.49982E+00 0.         0.         0.         0.         0.10830E+04

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Figure 6.   Iteration sequence and portion of output after time step 2.

RF1 ... EOS7-TEST: INJECT AIR, HEAT, BRINE AND FRESH WATER

OUTPUT DATA AFTER (52, 5)-2-TIME STEPS   THE TIME IS 0.100000E+01 DAYS

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TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
0.864000E+05	52	5	271	2	0.31302E+05	0.47029E-01	0.64245E-01	0.19466E-07	21	1	0.26880E+04

0@@@

OELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XBRINE(LIQ)	XAIRG	XAIRL	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
A11 1	1	0.39334E+06	0.10330E+03	0.65235E-01	0.93476E+00	0.52361E+00	0.79505E+00	0.28542E-04	-.40772E+05	0.32525E+01	0.10424E+04
A21 1	2	0.46677E+06	0.10676E+03	0.57646E-01	0.94235E+00	0.41642E+00	0.80625E+00	0.38910E-04	-.36029E+05	0.38484E+01	0.10207E+04
A12 1	3	0.48283E+06	0.10277E+03	0.79610E-01	0.92039E+00	0.42418E+00	0.83995E+00	0.42324E-04	-.49757E+05	0.40933E+01	0.10253E+04
A22 1	4	0.50510E+06	0.14350E+03	0.79769E-01	0.92023E+00	0.29570E+00	0.29207E+00	0.13719E-04	-.49856E+05	0.30464E+01	0.96820E+03
A13 1	5	0.52397E+06	0.86828E+02	0.94582E-01	0.90542E+00	0.45732E+00	0.92204E+00	0.50867E-04	-.59114E+05	0.48471E+01	0.10431E+04
A23 1	6	0.54844E+06	0.15150E+03	0.11606E+00	0.88394E+00	0.25307E+00	0.14119E+00	0.70894E-05	-.72537E+05	0.30808E+01	0.95368E+03
A14 1	7	0.54799E+06	0.28650E+02	0.92845E-01	0.90716E+00	0.69116E+00	0.99553E+00	0.44101E-04	-.58028E+05	0.63073E+01	0.11190E+04
A24 1	8	0.55699E+06	0.55054E+02	0.91878E-01	0.90812E+00	0.35949E+00	0.98211E+00	0.65815E-04	-.57423E+05	0.58482E+01	0.10455E+04
A15 1	9	0.55951E+06	0.25119E+02	0.92486E-01	0.90751E+00	0.95607E+00	0.99644E+00	0.25066E-04	-.57804E+05	0.65197E+01	0.11756E+04
A25 1	10	0.57128E+06	0.26811E+02	0.93387E-01	0.90661E+00	0.43833E+00	0.99615E+00	0.63807E-04	-.58367E+05	0.66181E+01	0.10714E+04
A11 2	11	0.47108E+06	0.12742E+03	0.54232E-01	0.94577E+00	0.69536E+00	0.58015E+00	0.17805E-04	-.33895E+05	0.33145E+01	0.10530E+04
A21 2	12	0.49637E+06	0.12764E+03	0.55512E-01	0.94449E+00	0.54728E+00	0.60307E+00	0.24289E-04	-.34695E+05	0.35275E+01	0.10257E+04
A12 2	13	0.55925E+06	0.15608E+03	0.15789E+00	0.84211E+00	0.47719E+00	0.13197E-02	0.52004E-07	-.98682E+05	0.29677E+01	0.98563E+03
A22 2	14	0.63604E+06	0.16113E+03	0.26078E+00	0.73922E+00	0.36817E+00	0.97222E-05	0.48970E-09	-.16299E+06	0.33495E+01	0.96233E+03
A13 2	15	0.62725E+06	0.16058E+03	0.24009E+00	0.75991E+00	0.40369E+00	0.20796E-03	0.99713E-08	-.15006E+06	0.33060E+01	0.96871E+03
A23 2	16	0.73147E+06	0.16674E+03	0.39024E+00	0.60976E+00	0.17388E+00	0.36461E-07	0.25068E-11	-.24390E+06	0.38233E+01	0.92613E+03
A14 2	17	0.55409E+06	0.61082E+02	0.89555E-01	0.91045E+00	0.56224E+00	0.97602E+00	0.51916E-04	-.55972E+05	0.56925E+01	0.10790E+04
A24 2	18	0.63197E+06	0.16087E+03	0.20418E+00	0.79582E+00	0.14062E+00	0.34351E-03	0.20805E-07	-.12761E+06	0.33296E+01	0.92708E+03
A15 2	19	0.55901E+06	0.26136E+02	0.78483E-01	0.92152E+00	0.84785E+00	0.99622E+00	0.33441E-04	-.49052E+05	0.64908E+01	0.11520E+04
A25 2	20	0.56668E+06	0.43265E+02	0.73611E-01	0.92639E+00	0.21474E+00	0.99030E+00	0.76948E-04	-.46007E+05	0.62016E+01	0.10261E+04
A11 3	21	0.55593E+06	0.15578E+03	0.11884E+00	0.88116E+00	0.91888E+00	0.38488E-02	0.70460E-07	-.74273E+05	0.29539E+01	0.10668E+04
A21 3	22	0.53052E+06	0.13661E+03	0.58228E-01	0.94177E+00	0.67770E+00	0.48942E+00	0.16766E-04	-.36392E+05	0.35170E+01	0.10408E+04
A12 3	23	0.63557E+06	0.16110E+03	0.23473E+00	0.76527E+00	0.63633E+00	0.17309E-03	0.63634E-08	-.14671E+06	0.33474E+01	0.10079E+04
A22 3	24	0.72330E+06	0.16628E+03	0.35804E+00	0.64196E+00	0.46788E+00	0.23394E-04	0.12155E-08	-.22377E+06	0.37828E+01	0.97327E+03
A13 3	25	0.71853E+06	0.16601E+03	0.35609E+00	0.64391E+00	0.35582E+00	0.86864E-04	0.50245E-08	-.22256E+06	0.37593E+01	0.95522E+03
A23 3	26	0.93376E+06	0.17693E+03	0.70504E+00	0.29496E+00	0.44942E+01	0.82030E-08	0.82150E-13	-.44065E+06	0.48214E+01	0.30985E+04
A14 3	27	0.55833E+06	0.13318E+03	0.81875E-01	0.91813E+00	0.36201E+00	0.57814E+00	0.31718E-04	-.51172E+05	0.38763E+01	0.98874E+03
A24 3	28	0.71046E+06	0.16555E+03	0.30813E+00	0.69187E+00	0.33497E+01	0.14767E-03	0.10881E-07	-.19258E+06	0.37194E+01	0.90660E+03
A15 3	29	0.55756E+06	0.30539E+02	0.56274E-01	0.94373E+00	0.52837E+00	0.99510E+00	0.56172E-04	-.35171E+05	0.63758E+01	0.10869E+04
A25 3	30	0.56472E+06	0.87503E+02	0.54052E-01	0.94595E+00	0.41516E-01	0.92590E+00	0.78382E-04	-.33782E+05	0.52257E+01	0.97343E+03
A11 4	31	0.66388E+06	0.16283E+03	0.23305E+00	0.76695E+00	0.11735E+01	0.	0.	-.14566E+06	0.34879E+01	0.11113E+04
A21 4	32	0.55613E+06	0.13675E+03	0.54696E-01	0.94530E+00	0.87281E+00	0.51676E+00	0.12872E-04	-.34185E+05	0.37296E+01	0.10781E+04
A12 4	33	0.56471E+06	0.13630E+03	0.81581E-01	0.91842E+00	0.85158E+00	0.53378E+00	0.14301E-04	-.50988E+05	0.38191E+01	0.10744E+04
A22 4	34	0.56590E+06	0.14821E+03	0.70431E-01	0.92957E+00	0.49109E+00	0.27600E+00	0.11912E-04	-.44020E+05	0.33634E+01	0.99607E+03
A13 4	35	0.56491E+06	0.13240E+03	0.74553E-01	0.92545E+00	0.34881E+00	0.59282E+00	0.33321E-04	-.46596E+05	0.39299E+01	0.98727E+03
A23 4	36	0.70573E+06	0.16528E+03	0.29035E+00	0.70965E+00	0.75172E-01	0.12219E-03	0.86939E-08	-.18147E+06	0.36959E+01	0.91293E+03
A14 4	37	0.55773E+06	0.33759E+02	0.47202E-01	0.95280E+00	0.33942E+00	0.99411E+00	0.68461E-04	-.29502E+05	0.63071E+01	0.10513E+04
A24 4	38	0.53501E+06	0.12450E+03	0.	0.10000E+01	0.18539E-01	0.	0.39871E-04	0.	0.	0.94210E+03
A15 4	39	0.54756E+06	0.38411E+02	0.10292E-01	0.98971E+00	0.17768E+00	0.99225E+00	0.76777E-04	-.64325E+04	0.60928E+01	0.10219E+04
A25 4	40	0.55350E+06	0.63839E+02	0.	0.10000E+01	0.16474E-02	0.	0.39635E-04	0.	0.	0.98160E+03
A11 5	41	0.80134E+06	0.17048E+03	0.35431E+00	0.64569E+00	0.11624E+01	0.56127E-13	0.47906E-18	-.22145E+06	0.41688E+01	0.10995E+04
A21 5	42	0.68772E+06	0.16424E+03	0.22711E+00	0.77289E+00	0.10788E+01	0.71812E-10	0.88272E-15	-.14195E+06	0.36063E+01	0.10895E+04
A12 5	43	0.66813E+06	0.16309E+03	0.21327E+00	0.78673E+00	0.10844E+01	0.11867E-10	0.13717E-15	-.13329E+06	0.35091E+01	0.10920E+04
A22 5	44	0.55804E+06	0.97576E+02	0.29517E-01	0.97048E+00	0.70391E+00	0.88806E+00	0.36936E-04	-.18448E+05	0.49213E+01	0.10807E+04
A13 5	45	0.55643E+06	0.53735E+02	0.38852E-01	0.96115E+00	0.45408E+00	0.98320E+00	0.59855E-04	-.24283E+05	0.58697E+01	0.10631E+04

Figure 7.   TOUGH2 output after 1 day of simulation time.